

University of Groningen

Synthetic, Crystallographic, and Computational Study of Copper(II) Complexes of Ethylenediaminetetracarboxylate Ligands

Matovic, Zoran D.; Miletic, Vesna D.; Cendic, Marina; Meetsma, Auke; van Koningsbruggen, Petra J.; Deeth, Robert J.; Matović, Zoran D.; Miletić, Vesna D.; Čendić, Marina

Published in:
Inorganic Chemistry

DOI:
[10.1021/ic301609t](https://doi.org/10.1021/ic301609t)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2013

[Link to publication in University of Groningen/UMCG research database](#)

Citation for published version (APA):

Matovic, Z. D., Miletic, V. D., Cendic, M., Meetsma, A., van Koningsbruggen, P. J., Deeth, R. J., Matović, Z. D., Miletić, V. D., & Čendić, M. (2013). Synthetic, Crystallographic, and Computational Study of Copper(II) Complexes of Ethylenediaminetetracarboxylate Ligands. *Inorganic Chemistry*, 52(3), 1238-1247.
<https://doi.org/10.1021/ic301609t>

Copyright

Other than for strictly personal use, it is not permitted to download or to forward/distribute the text or part of it without the consent of the author(s) and/or copyright holder(s), unless the work is under an open content license (like Creative Commons).

The publication may also be distributed here under the terms of Article 25fa of the Dutch Copyright Act, indicated by the "Taverne" license. More information can be found on the University of Groningen website: <https://www.rug.nl/library/open-access/self-archiving-pure/taverne-amendment>.

Take-down policy

If you believe that this document breaches copyright please contact us providing details, and we will remove access to the work immediately and investigate your claim.

Downloaded from the University of Groningen/UMCG research database (Pure): <http://www.rug.nl/research/portal>. For technical reasons the number of authors shown on this cover page is limited to 10 maximum.

Supporting Information Available: CCDC 891689 contain the supplementary crystallographic data. These data can be obtained free of charge via <http://www.ccdc.cam.ac.uk/conts/retrieving.html>, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK; fax: (+44) 1223-336-033; or e-mail: deposit@ccdc.cam.ac.uk. Structural data for Ba[Cu(eda3p)]·8H₂O considered herein (Table S1), conformations of *N*-membered rings (Table S2) and data of IR spectra of Cu-edta-type of complexes (Table S3).

Table S1. Structural data for Ba[Cu(eda3p)]·8H₂O

M-L bond lengths (Å)			
Cu-O1	1.9514(17)		
Cu-O3	2.5180(17)		
Cu-O5	2.2994(16)		
Cu-O7	2.0130(16)		
Cu-N1	2.026(2)		
Cu-N2	2.022(2)		
M-O-C angles (°)			
Cu-O1-C1	128.12(16)		
Cu-O3-C6	100.24(15)		
Cu-O7-C13	113.05(14)		
Cu-O5-C11	108.27(15)		
Bond angles (°)			
<i>Cis</i> angles		<i>Trans</i> angles	
O3-Cu-O7	79.26(6)	O1-Cu-N2	174.67(8)
O3-Cu-N1	86.80(7)	O3-Cu-O5	166.68(5)
O3-Cu-N2	95.42(7)	O7-Cu-N1	162.46(9)
O5-Cu-O7	89.38(6)		
O5-Cu-N1	105.59(7)		
O5-Cu-N2	89.88(7)		
O7-Cu-N2	82.32(7)		
N1-Cu-N2	88.51(9)		
O7-Cu-O1	97.11(7)		
O3-Cu-O1	89.66(6)		
O5-Cu-O1	84.82(7)		
O1-Cu-N1	93.37(9)		

Table S2. Conformations of N -membered Rings ($N \leq 8$)

Ring Size N	Definition	Descriptive Name	Descriptive Symbol
4	$q_2 \neq 0$	puckered form	
5	$q_2 > 0; \phi_2 = 0$	envelope	
	$q_2 > 0; \phi_2 = \pi/2$	twist form	
6	$q_3 = 0; q_2 > 0; \phi_2 = 0$	boat	
	$q_3 = 0; q_2 > 0; \phi_2 = \pi/2$	twist-boat	
	$q_2 = 0; q_3 \neq 0$	chair	
7	$q_3 = 0; q_2 > 0; \phi_2 = 0$	boat	
	$q_3 = 0; q_2 > 0; \phi_2 = \pi/2$	twist-boat	
	$q_2 = 0; q_3 > 0; \phi_3 = 0$	chair	
	$q_2 = 0; q_3 > 0; \phi_3 = \pi/2$	twist-chair	
8	$q_4 = q_3 = 0; q_2 > 0; \phi_2 = 0$	boat-boat	
	$q_4 = q_3 = 0; q_2 > 0; \phi_2 = \pi/2$	twist-boat	
	$q_4 = q_2 = 0; q_3 > 0; \phi_3 = 0$	long-chair	
	$q_4 = q_2 = 0; q_3 > 0; \phi_3 = \pi/2$	twist-chair	
	$q_3 = q_2 = 0; q_4 \neq 0$	crown	

Table S3. Data of IR spectra of Cu-edta-type of complexes

Complex	Vibration (cm ⁻¹) v _{asym} (COOM)	Chelate ring size	Reference
<i>trans</i> (O ₅)-[BaCu(edta)(H ₂ O) ₃]·H ₂ O	1600	5	*
<i>trans</i> (O ₅)-Mg[Cu(ed3ap)]·8H ₂ O	1683	5	This work
	1598	6	
<i>trans</i> (O ₅)-Ba[Cu(edd3ap)]·8H ₂ O	1598	5 and 6	This work
<i>trans</i> (O ₆)-Ba[Cu(eda3p)]·8H ₂ O	1575	6	This work
	1623	5	
[Mg(H ₂ O) ₅][Cu(edtp)]	1572	6	(35)

*Insausti, M.; Pizarro, J. L.; Lezama, L.; Cortes, R.; Bocanegra, E. H.; Arriortua, M. I.; Rojo, T. *Chem. Mater.* **1994**, *6*, 707-713.